Integrating Computational and Organic Chemistry: Impacts of a Short-Term Activity on Imagistic Thinking and Epistemological Development in First-Semester Organic Chemistry Students

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Introduction

- Organic chemistry requires the use of spatial skills.[2] Students rely on imagistic thinking, while experts use analytical approaches.[2, 6] The transition between these spatial approaches is essential but under-supported.[1,3,11,13]
- Computational chemistry offers the ability to build interactive 3D visualization that can enhance spatial reasoning by scaffolding imagistic thinking skills.[1]
- Epistemologically sophisticated students have been shown to have stronger learning outcomes.[7]
- Objective of the research is to investigate how Integrating computational chemistry into organic chemistry curricula affects students necessary spatial thinking skills, and epistemological beliefs.

Research Questions

- RQ1: Does the use of computational methods to model chemical phenomena support the development of Imagistic thinking skills
- RQ2: Can a short-term intervention using multiple models of representation, and refutational texts promote students epistemological beliefs from naive to complex
- RQ3: Can this activity act as an exemplar to support the island of computation approach, so instructors, regardless of their computational skills, can implement pre-made modules into their courses

Epistemology

- Epistemology is a theory of the nature and justification of human knowledge
- Perry's Scheme: Stages of Sophistication.[5,12]
  - Limitation of scheme: commitment within relativism, originally discussed as a qualitative model, rather than a developmental stage. Also detracts from knowledge and speaks to ethical development

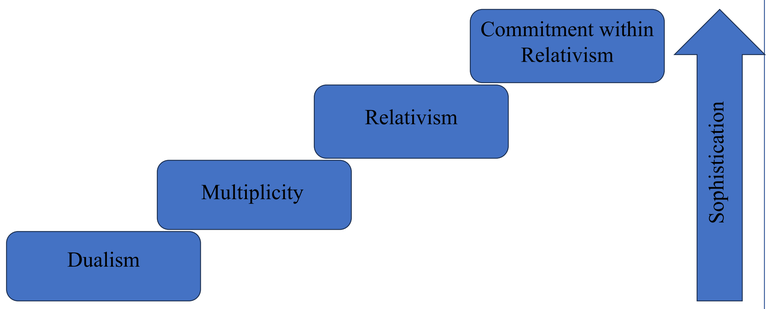

Figure 1: Levels of epistemological sophistication, beginning from naïve and increasing in complexity

Spatial Thinking

- Spatial thinking is the ability to think about physical and imagined spatial relationships.[2]
- Imagistic thinking is the process of generating mental imagery, manipulating said imagery, and perspective taking.[6]
- Analytical thinking is an algorithmic or heuristic approach which uses rules to efficiently think about spatial problems.[2,6]
- As students gain experience they progress from using imagistic thinking to increasing use of analytical thinking.[11]

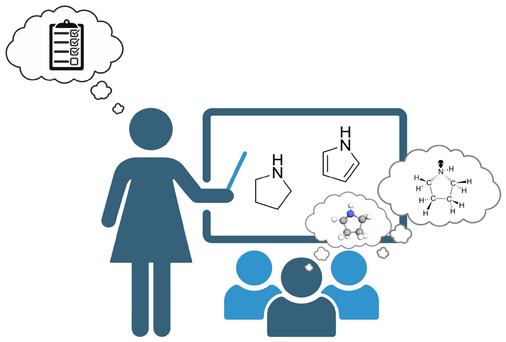

Figure 2: Differences in application of spatial thinking skills, where experts use analytical thinking, and students use imagistic thinking (symbols should be thought of in a 3D space) Created with BioRender.com, ChemDraw, and Molview.org

- Physical models offer a more direct approach to scaffolding spatial skills.[3]
  - Areas to be addressed: no training provided to virtual media, virtual structures were not made by students- only manipulated
- Virtual models allow more opportunities to link 2D and 3D representations.[1]
- Scaffolding spatial thinking: showing multiple representations, the transformation from 2D images to 3D images.[13]

3 Models of Integration[10]

- Specialized courses: An elective computational chemistry-based course
- Augmented courses: Degree requirement courses that teach core concepts through the use of computational methods
- Islands of Computation: Application of modules to teach concepts, through computational methods, within traditional courses

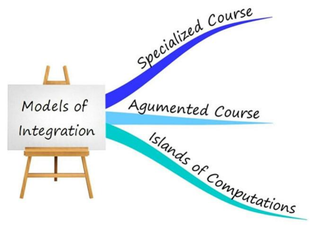

Figure 3: Graphic of the different models of integrating computational chemistry into undergraduate curricula.[10]

Methods and Materials

- Method
  - Quantitative Data
    - Pre- and Post-tests of Spatial skills using the Vandenberg Mental Rotation Test.[9]
    - Pre- and post-test of students epistemological beliefs
  - Statistical method
    - Latent profile analysis will be used to address sub-group classifications that can be made within Perry's Scheme.[8]
  - Qualitative data.[4]
    - Unstructured-Observation of class setting using video and audio recording
    - Open responses from students
    - Instructor account
- Material: Virtual activity
  - Students will use code provided to them, to generate orbitals, hybridized orbitals, and molecular geometries of molecules
  - As students progress through the activity, they must select code based on the desired representational model (i.e. 2D, 3D static, 3D interactive) for each section (orbitals, hybridized orbitals, molecular geometries).
  - Open response will be obtained after code sections, so students practice questioning their belief of knowledge.

Expected Findings (possible implications)

- A successful module will be operable regardless of the instructor's background in computational methods, indicating that the island of computation may be the most assessable means to introduce undergraduate students to the discipline of computational chemistry.
- Discovering if multiple models of representations through a virtual medium along with students reflecting on their knowledge generation process supports epistemological promotion. This can give us insight in how we can embed epistemic practices into our lesson plans.
- Understanding if imagistic thinking skills through, virtual mediums, can be scaffolded by students generating their own interactive visuals. This can provide students with more tools to practice imagistic thinking while gaining domain-specific expertise as they transition to relying on analytical thinking.
- Revisiting Perry's Scheme by evaluating what type of sub-groups exist in his original framework may show some insights into the application across differing cultures.
- Greater focus on epistemology in the context of chemistry curricula in higher education will enable us to learn how to support students' domain-specific epistemological beliefs

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References

1. Abraham, M.; Varghese, V.; Tang, H. Using Molecular Representations To Aid Student Understanding of Stereochemical Concepts. *J. Chem. Educ.* **2010**, *87* (12), 1425–1429. https://doi.org/10.1021/ed100497f.
2. Atit, K.; Uttal, D. H.; Stieff, M. Situating Space: Using a Discipline-Focused Lens to Examine Spatial Thinking Skills. *Cogn. Res. Princ. Implic.* **2020**, *5*, 19. https://doi.org/10.1186/s41235-020-00210-z.
3. Casselman, M. D.; Eichler, J. F.; Atit, K. Advancing Multimedia Learning for Science: Comparing the Effect of Virtual versus Physical Models on Student Learning about Stereochemistry. *Sci. Educ.* **2021**, *105* (6), 1285–1314. https://doi.org/10.1002/sce.21675.
4. Cohen, L.; Manion, L.; Morrison, K. *Research Methods in Education*, 6th ed.; Routledge: London ; New York, 2007.
5. Hofer, B. K.; Pintrich, P. R. The Development of Epistemological Theories: Beliefs about Knowledge and Knowing and Their Relation to Learning. *Rev. Educ. Res.* **1997**, *67* (1), 88–140. https://doi.org/10.2307/1170620.
6. Kienhues, D.; Bromme, R.; Stahl, E. Changing Epistemological Beliefs: The Unexpected Impact of a Short-Term Intervention: British Journal of Educational Psychology. *Br. J. Educ. Psychol.* **2008**, *78* (4), 545–565. https://doi.org/10.1348/000709907X268589.
7. Kiernan, N. A.; Manches, A.; Seery, M. K. The Role of Visuospatial Thinking in Students' Predictions of Molecular Geometry. *Chem. Educ. Res. Pract.* **2021**, *22* (3), 626–639. https://doi.org/10.1039/D0RP00354A.
8. Mathew, A.; Doorenbos, A. Z. Latent Profile Analysis – An Emerging Advanced Statistical Approach to Subgroup Identification. *Indian J. Contin. Nurs. Educ.* **2022**, *23* (2), 127. https://doi.org/10.4103/ijcn.ijcn_24_22.
9. Stieff, M.; Ryu, M.; Dixon, B.; Hegarty, M. The Role of Spatial Ability and Strategy Preference for Spatial Problem Solving in Organic Chemistry. *J. Chem. Educ.* **2012**, *89* (7), 854–859. https://doi.org/10.1021/ed200071d.
10. Truvi-Arad, I. Computational Chemistry in the Undergraduate Classroom – Pedagogical Considerations and Teaching Challenges. *Isr. J. Chem.* **2022**, *62* (1/2), 1–9. https://doi.org/10.1002/ijch.202100042.
11. Vlacholia, M.; Vosniadou, S.; Roussos, P.; Salta, K.; Kazi, S.; Sigalas, M.; Tzougraki, C. Changes in Visual/Spatial and Analytic Strategy Use in Organic Chemistry with the Development of Expertise. *Chem. Educ. Res. Pract.* **2017**, *18* (4), 763–773. https://doi.org/10.1039/C7RP00036G.
12. William, P.; Knefelkamp, L. *Forms of Ethical and Intellectual Development in the College Years: A Scheme*, First.; Jossey-Bass A Wiley Company, 1999.
13. Wu, H.-K.; Shah, P. Exploring Visuospatial Thinking in Chemistry Learning. *Sci. Educ.* **2004**, *88* (3), 465–492. https://doi.org/10.1002/sce.10126.